Integral circulant graphs of prime power order with maximal energy

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Abstract

The energy of a graph is the sum of the moduli of the eigenvalues of its adjacency matrix. We study the energy of integral circulant graphs, also called gcd graphs, which can be characterized by their vertex count n and a set $\mathcal{D}$ of divisors of n in such a way that they have vertex set $\mathbb{Z}_n$ and edge set $\{\{a,b\} : a, b \in \mathbb{Z}_n, \gcd(a-b,n) \in \mathcal{D}\}$. Using tools from convex optimization, we study the maximal energy among all integral circulant graphs of prime power order p^s and varying divisor sets $\mathcal{D}$. Our main result states that this maximal energy approximately lies between $s(p-1)p^{s-1}$ and twice this value. We construct suitable divisor sets for which the energy lies in this interval. We also characterize hyperenergetic integral circulant graphs of prime power order and exhibit an interesting topological property of their divisor sets.

1   Introduction

Concerning the energies of integral circulant graphs, an interesting open problem is the characterization of those graphs having maximal energy among all integral circulant graphs with the same given number of vertices. The goal of this paper is to establish clarity concerning this question, for integral circulant graphs of prime power order, by showing how to construct such graphs with a prescribed number of vertices whose energy comes close to the desired maximum. In the course of this, we approximately determine the maximal energy itself. We rely on a closed formula for the energy of an integral circulant graph with prime power order that was established in [18].

A circulant graph is a graph whose adjacency matrix (with respect to a suitable vertex indexing) can be constructed from its first row by a process of continued rotation of entries. An integral circulant graph is a circulant graph whose adjacency matrix has only integer eigenvalues. The integral circulant graphs belong to the class of Cayley graphs. By a result of So [20], they are in fact exactly the class of the so-called gcd graphs [20], a class that originally arose as a generalization of unitary Cayley graphs. The gcd graphs have first been described by KLOTZ and SANDER in [10] and further studied e.g. by BAŠIĆ and ILIĆ [3], [7]. The way the gcd graphs are defined serves us well, so throughout this paper we shall make use of this particular perspective of perceiving integral circulant graphs. Given an integer n and a set $\mathcal{D}$ of positive divisors of n, the integral circulant graph $\mathrm{ICG}(n, \mathcal{D})$ is defined as the corresponding gcd graph having vertex set $\mathbb{Z}_n = \{0, 1, \ldots, n-1\}$ and edge set $\{\{a, b\} : a, b \in \mathbb{Z}_n, \gcd(a - b, n) \in \mathcal{D}\}$. We consider only loopfree gcd graphs, i.e. $n \notin \mathcal{D}$.

The *energy* $E(G)$ of a graph G on n vertices is defined as

$$E(G) = \sum_{i=1}^{n} |\lambda_i|,$$

where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix of G. This concept has been introduced several decades ago by GUTMAN [5], and with slight modification it can even be extended to arbitrary real rectangular matrices, cf. [13] and [9].

There exist many bounds for the graph energy, see BRUALDI [4] for a short survey. One example is the bound

$$E(G) \leq \frac{n}{2} \left(\sqrt{n} + 1 \right)$$

due to KOOLEN and MOULTON [11] for any graph with n vertices. There exist infinitely many graphs that achieve this bound. If we consider only the class of circulant graphs, then the question arises how close one can get to this bound. SHPARLINKSI [19] has given an explicit construction of an infinite family of graphs that asymptotically achieves the bound.

Another well-known result is due to BALAKRISHNAN, who gives an upper bound $B = k + \sqrt{k(n-1)(n-k)}$ for the energy of a k-regular graph on n vertices (see [2]). LI ET AL. [12] have shown that for every $\varepsilon > 0$ one can actually find infinitely many k-regular graphs G such that $\frac{E(G)}{B} > 1 - \varepsilon$.

There has been some recent work on the energy of unitary Cayley graphs, which are exactly the gcd graphs with $\mathcal{D} = \{1\}$. Let us abbreviate $\mathcal{E}(n, \mathcal{D}) = E(\mathrm{ICG}(n, \mathcal{D}))$ and let $n = p_1^{s_1} \cdots p_k^{s_k}$. Then, in the context of gcd graphs, the following result has been obtained by RAMASWAMY and VEENA [14] and, independently, by ILIĆ [7]:

$$\mathcal{E}(n, \{1\}) = 2^k \varphi(n),$$

where φ denotes Euler's totient function.

ILIĆ [7] has slightly generalized this to some gcd graphs that are not unitary Cayley graphs:

$$\begin{aligned}
\mathcal{E}(n, \{1, p_i\}) &= 2^{k-1} p_i \varphi(n/p_i), &&\text{provided that } s_i = 1, \\
\mathcal{E}(n, \{p_i, p_j\}) &= 2^k \varphi(n), &&\text{provided that } s_1 = \ldots = s_k = 1.
\end{aligned}$$

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In [18] the authors proved an explicit formula for the energy of $\text{ICG}(p^s, \mathcal{D})$ for any prime power p^s and any divisor set $\mathcal{D} = \{p^{a_1}, p^{a_2}, \ldots, p^{a_r}\}$ with $0 \leq a_1 < a_2 < \ldots < a_r \leq s-1$, namely

$$\mathcal{E}(p^s, \mathcal{D}) = 2(p-1)\left(p^{s-1}r - (p-1)\sum_{k=1}^{r-1}\sum_{i=k+1}^{r} p^{s-a_i+a_k-1}\right). \tag{1}$$

The study of energies is usually linked to the search for hyperenergetic graphs. A graph G on n vertices is called *hyperenergetic* if its energy is greater than the energy of the complete graph on the same number of vertices, i.e. if $E(G) > E(K_n) = 2(n-1)$. Initially, the existence of hyperenergetic graphs had been doubted, but then more and more classes of hyperenergetic graphs were discovered. For example, HOU and GUTMAN show in [6] that if a graph G has more than $2n-1$ edges, then its line graph $L(G)$ is necessarily hyperenergetic. Consequently, $L(K_n)$ is hyperenergetic for all $n \geq 5$, a fact that seems to have been known before.

Work by STEVANOVIĆ and STANKOVIĆ [21] indicates that the class of circulant graphs contains a wealth of hyperenergetic graphs. Although integral circulant graphs are quite rare among circulant graphs (cf. [1]), the subclass of integral circulant graphs still exhibits many hyperenergetic members. For example, it has been shown by RAMASWAMY and VEENA [14] that almost all unitary Cayley graphs on n vertices are hyperenergetic. The necessary and sufficient condition is that n has at least 3 distinct prime divisors or that n is odd in case of only two prime divisors. Consequently, there exist no gcd graphs $\text{ICG}(p^s, \mathcal{D})$ with $\mathcal{D} = \{1\}$ that are hyperenergetic. However, for less trivial divisor sets it is also possible to find hyperenergetic gcd graphs on p^s vertices. Some examples are given in [18]. For instance, for $p \geq 3$ and $s \geq 3$, the choice $\mathcal{D} = \{1, p^{s-1}\}$ yields a hyperenergetic gcd graph.

Not surprisingly, the class of graphs $\text{ICG}(p^s, \mathcal{D})$ contains also non-hyperenergetic elements, termed *hypoenergetic*. For the minimal energy $\mathcal{E}_{\min}(n)$ of all integral circulant graphs with n vertices it has been shown in [18] that

$$\mathcal{E}_{\min}(p^s) = 2(p-1)p^{s-1} = E(K_{p^s}) - E(K_{p^{s-1}}).$$

This follows directly from equation (1). The minimal energy is achieved exactly for the singleton divisor sets.

The maximum energy of graphs $\text{ICG}(p^s, \mathcal{D})$ is not as easily described. A classification of integral circulant graphs of prime power order p^s with very small exponent having maximal energy has been provided in [18], but it became clear that a general result as simple as in the case of minimal energy could not be expected. It will be the purpose of this article to clarify the structure of divisor sets imposing maximal energy on the corresponding gcd graph. Our main Theorem 4.2 states that the maximal energy among all integral circulant graphs of prime power order p^s and varying divisor sets $\mathcal{D}$ approximately lies between $s(p-1)p^{s-1}$ and twice this value. Tools from convex optimization will turn out to be the appropriate machinery to reach that goal. We shall compute bounds for the maximum energy and describe how to construct divisor sets for integral circulant graphs on p^s vertices that have

near maximal energy. Along the way, we characterize hyperenergetic integral circulant graphs of prime power order and exhibit an interesting topological property of their divisor sets. Namely, the set containing all ordered exponent tuples corresponding to these divisor sets can be obtained by intersecting an integer grid with a suitable convex set.

2 Preliminary definitions and results

For any positive integer n, let

$$\mathcal{E}_{\max}(n) := \max\left\{\mathcal{E}(n, \mathcal{D}) : \mathcal{D} \subseteq \{1 \leq d < n : d \mid n\}\right\}.$$

For given $\mathcal{D} = \{p^{a_1}, p^{a_2}, \ldots, p^{a_r}\}$ with $0 \leq a_1 < \ldots < a_r \leq s - 1$, we have by (1), i.e. by Theorem 2.1 in [18], that

$$\mathcal{E}(p^s, \mathcal{D}) = 2(p - 1)p^{s-1}(r - (p - 1)h_p(a_1, \ldots, a_r)), \tag{2}$$

where

$$h_p(x_1, \ldots, x_r) := \sum_{k=1}^{r-1} \sum_{i=k+1}^{r} \frac{1}{p^{x_i - x_k}}$$

for arbitrary real numbers $x_1, \ldots, x_r$. In order to evaluate $\mathcal{E}_{\max}(p^s)$, our main task will be to determine

$$\mathcal{E}_{\max}(p^s, r) := \max\left\{\mathcal{E}(p^s, \mathcal{D}) : \mathcal{D} \subseteq \{1 \leq d < n : d \mid n\}, |\mathcal{D}| = r\right\}$$

as precisely as possible, given a fixed integer r. Therefore, we define for $1 \leq r \leq s + 1$

$$m_p(s, r) := \min\left\{h_p(a_1, \ldots, a_r) : 0 \leq a_1 < a_2 < \ldots < a_r \leq s \text{ with } a_i \in \mathbb{Z}\right\}. \tag{3}$$

It is then clear from (2) that

$$\mathcal{E}_{\max}(p^s, r) = 2(p - 1)p^{s-1}(r - (p - 1)m_p(s - 1, r)). \tag{4}$$

Later on it remains to compute

$$\mathcal{E}_{\max}(p^s) = \max\left\{\mathcal{E}_{\max}(p^s, r) : 1 \leq r \leq s\right\}. \tag{5}$$

Proposition 2.1 *Let p be a prime. Then*

(i) $m_p(s, 2) = \frac{1}{p^s}$ *for all integers $s \geq 1$, and the minimum is attained only for $a_1 = 0$ and $a_2 = s$.*

(ii) $m_p(s, 3) = \frac{1}{p^{[s/2]}} + \frac{1}{p^s} + \frac{1}{p^{s-[s/2]}}$ *for all integers $s \geq 2$. The minimum is only obtained for $a_1 = 0$, $a_2 = [s/2]$ (or, additionally, for $a_2 = [s/2] + 1$ if s is odd) and $a_3 = s$.*

PROOF.   Proposition 3.1 in [18].

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□

A set $\mathcal{D} \subseteq \{1 \leq d < n : d \mid n\}$ is called *n-maximal* if $\mathcal{E}(n, \mathcal{D}) = \mathcal{E}_{\max}(n)$. As a consequence of Proposition 2.1 and some other results in [18], we obtained

Theorem 2.1 *Let p be a prime. Then*

(i) $\mathcal{E}_{\max}(p) = 2(p-1)$ *with the only p-maximal set $\mathcal{D} = \{1\}$.*

(ii) $\mathcal{E}_{\max}(p^2) = 2(p-1)(p+1)$ *with the only p^2-maximal set $\mathcal{D} = \{1, p\}$.*

(iii) $\mathcal{E}_{\max}(p^3) = 2(p-1)(2p^2 - p + 1)$ *with the only p^3-maximal set $\mathcal{D} = \{1, p^2\}$, except for the prime $p = 2$ for which $\mathcal{D} = \{1, 2, 4\}$ is also 2^3-maximal.*

(iv) $\mathcal{E}_{\max}(p^4) = 2(p-1)(2p^3 + 1)$ *with the only p^4-maximal sets $\mathcal{D} = \{1, p, p^3\}$ and $\mathcal{D} = \{1, p^2, p^3\}$.*

PROOF. Theorem 3.2 in [18].

□

One can prove formulae for $\mathcal{E}_{\max}(p^s)$ with arbitrary exponent s by using (4) and (5). As indicated in Proposition 2.1, we need to choose integers $0 \leq a_1 \leq a_2 \leq \ldots \leq a_r \leq s - 1$ in such a way that

$$h_p(a_1, \ldots, a_r) = \sum_{k=1}^{r-1} \sum_{i=k+1}^{r} \frac{1}{p^{a_i - a_k}}$$

becomes minimal. The choice of $a_1 = 0$ and $a_r = s - 1$ is clearly compulsory.

The case $r = 3$ (cf. Prop. 2.1(ii)) suggests to place $a_1, a_2, \ldots, a_{r-1}, a_r$ equidistant in the interval $[0, s-1]$. A minor obstacle is the fact that the corresponding choice $a_i := \frac{(i-1)(s-1)}{r-1}$ $(1 \leq i \leq r)$ does not yield integral numbers as required. Taking nearest integers easily resolves this problem, but only at the cost of approximate instead of exact formulae. More seriously, it turns out that in general, even allowing real a_i, their equidistant positioning does not yield the desired minimum $m_p(s, r)$. The cases presented in Proposition 2.1 do not yet exhibit this problem since it makes its debut for $r = 4$. An illuminating example can be found in the final section of [18].

For the sake of being able to use analytic methods, we define for a prime p, a positive real number σ and a positive integer r

$$\tilde{m}_p(\sigma, r) := \min \{h_p(\alpha_1, \ldots, \alpha_r) : 0 \leq \alpha_1 \leq \alpha_2 \leq \ldots \leq \alpha_r \leq \sigma, \ \alpha_i \in \mathbb{R}\}. \tag{6}$$

Observe that now the α_i may be real numbers as opposed to integers in the definition of $m_p(s, r)$. It is obvious that for $r \geq 2$

$$\tilde{m}_p(\sigma, r) = \min \{h_p(0, \alpha_2, \ldots, \alpha_{r-1}, \sigma) : 0 \leq \alpha_2 \leq \ldots \leq \alpha_{r-1} \leq \sigma, \ \alpha_i \in \mathbb{R}\}. \tag{7}$$

Clearly, $\tilde{m}_p(\sigma, 2) = 1/p^\sigma$, uniquely obtained for $\alpha_1 = 0, \alpha_2 = \sigma$, and $\tilde{m}_p(\sigma, 3) = 1/p^\sigma + 2/p^{\sigma/2}$, uniquely obtained for $\alpha_1 = 0, \alpha_2 = \sigma/2, \alpha_3 = \sigma$ (cf. Proposition 2.1(ii)).

3 Tools from convex optimization

In order to determine $\tilde{m}_p(\sigma, r)$ in general it is crucial to observe that $h_p(x_1, \ldots, x_r)$ is a convex function.

Proposition 3.1 *Let r be a fixed positive integer, $b \neq 1$ a fixed positive real number and p a fixed prime.*

   (i) *The real function*

$$g_b(y_1, \ldots, y_r) := \sum_{k=1}^{r} \sum_{i=k}^{r} \prod_{j=k}^{i} \frac{1}{b^{y_j}}$$

    is strictly convex on $\mathbb{R}^r$.

  (ii) *The function $h_p(x_1, \ldots, x_r)$ is convex on $\mathbb{R}^r$.*

    PROOF.

(i) Let $(u_1, \ldots, u_r) \neq (v_1, \ldots, v_r)$ be arbitrary real vectors. On setting

$$U_{k,i} := \prod_{j=k}^{i} \frac{1}{b^{u_j}} \quad \text{and} \quad V_{k,i} := \prod_{j=k}^{i} \frac{1}{b^{v_j}},$$

we have $U_{k,k} = b^{-u_k}$ and $V_{k,k} = b^{-v_k}$ for $1 \leq k \leq r$. Since $0 < b \neq 1$ and $u_k \neq v_k$ for at least one k, we have $U_{k,k} \neq V_{k,k}$ for that k. By the inequality between the weighted arithmetic and the weighted geometric mean, which is an immediate consequence of Jensen's inequality (cf. [15], p. 1100, Thms. 17 and 18), we have $U^t \cdot V^{1-t} \leq tU + (1-t)V$ for all positive real numbers U and V and all $0 < t < 1$, with equality if and only if $U = V$. It follows that for all $1 \leq k \leq i \leq r$

$$U_{k,i}^t V_{k,i}^{1-t} \leq tU_{k,i} + (1-t)V_{k,i},$$

and strict inequality for at least one pair k, i. Hence

$$
\begin{aligned}
g_b\big(t(u_1, \ldots, u_r) + (1-t)(v_1, \ldots, v_r)\big) &= \sum_{k=1}^{r} \sum_{i=k}^{r} U_{k,i}^t V_{k,i}^{1-t} \\
&< \sum_{k=1}^{r} \sum_{i=k}^{r} tU_{k,i} + \sum_{k=1}^{r} \sum_{i=k}^{r} (1-t)V_{k,i} \\
&= tg_b(u_1, \ldots, u_r) + (1-t)g_b(v_1, \ldots, v_r).
\end{aligned}
$$

This proves that g is strictly convex on $\mathbb{R}^r$.

(ii) Let $(u_1, \ldots, u_r), (v_1, \ldots, v_r) \in \mathbb{R}^r$ and $0 < t < 1$. Then by (i)

$$
\begin{aligned}
h_p\big(t(u_1, \ldots, u_r) &+ (1-t)(v_1, \ldots, v_r)\big) = \\
&= g_p\big(t(u_2 - u_1, u_3 - u_2, \ldots, u_r - u_{r-1}) + (1-t)(v_2 - v_1, v_3 - v_2, \ldots, v_r - v_{r-1})\big) \\
&\leq tg_p\big(u_2 - u_1, u_3 - u_2, \ldots, u_r - u_{r-1}\big) + (1-t)g_p\big(v_2 - v_1, v_3 - v_2, \ldots, v_r - v_{r-1}\big) \\
&= th_p(u_1, \ldots, u_r) + (1-t)h_p(v_1, \ldots, v_r),
\end{aligned}
$$

which shows the convexity of h_p.

$\square$

An easy corollary of (1) is a characterisation of the hyperenergetic gcd graphs of prime power order, namely that $\mathrm{ICG}(p^s, \mathcal{D})$ with $\mathcal{D} = \{p^{a_1}, p^{a_2}, \ldots, p^{a_r}\}$ and $0 \le a_1 < a_2 < \ldots < a_r \le s - 1$ is hyperenergetic if and only if

$$\sum_{k=1}^{r-1} \sum_{i=k+1}^{r} \frac{1}{p^{a_i - a_k}} < \frac{1}{p-1}\left(r - \frac{p^s - 1}{p^{s-1}(p-1)}\right) \qquad (8)$$

(cf. Corollary 2.2 in [18]). As a first consequence of the convexity of h_p we are able to refine this by showing that the set of hyperenergetic integral circulant graphs has a nice topological feature. Given a prime p and positive integers $r \le s$, we define $\mathcal{H}(p^s, r)$ as the set containing all $(a_1, \ldots, a_r) \in \mathbb{Z}^r$ with $0 \le a_1 < \ldots < a_r \le s - 1$ and the property that $\mathrm{ICG}(p^s, \{p^{a_1}, \ldots, p^{a_r}\})$ is hyperenergetic. Then we can derive the following remarkable statement:

Corollary 3.1 *Let p be a prime and $r \le s$ positive integers. Then there is a convex set $C \subseteq \mathbb{R}^r$ such that $\mathcal{H}(p^s, r) = C \cap \mathbb{Z}^r$.*

PROOF. For fixed p, s and r, we define

$$c(p, s, r) := \frac{1}{p-1}\left(r - \frac{p^s - 1}{p^{s-1}(p-1)}\right).$$

Since h_p is convex on $\mathbb{R}^r$ by Proposition 3.1, the so-called level set

$$L := \{(x_1, \ldots, x_r) \in \mathbb{R}^r : h_p(x_1, \ldots, x_r) < c(p, s, r)\}$$

is also convex (cf. [17], p. 8 and Prop. 2.7). Since

$$K := \{(x_1, \ldots, x_r) \in \mathbb{R}^r : 0 \le x_1 < x_2 < \ldots < x_r \le s - 1\}$$

is obviously convex as well, the intersection $C := L \cap K$ has the same property. By (8) we know that some $(a_1, \ldots, a_r) \in \mathbb{Z}^r$ lies in $\mathcal{H}(p^s, r)$ if and only if $0 \le a_1 < \ldots < a_r \le s - 1$ and $h_p(a_1, \ldots, a_r) < c(p, s, r)$, hence $\mathcal{H}(p^s, r) = C \cap \mathbb{Z}^r$.
$\square$

We shall use some further standard results from convex optimization.

Proposition 3.2 *Let $f : U \to \mathbb{R}$ be a strictly convex function defined on a convex set $U \subseteq \mathbb{R}^r$.*

(i) If U is an open set then each extremal point of f is a minimum.

(ii) If f has a minimal point on U then it is unique.

PROOF. The proofs of the assertions can be found in [16], pp. 123-124, Theorems A and C, in [8], or in [17], Thm. 2.6.

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$\square$

Our main tool for the computation of $\tilde{m}_p(\sigma, r)$ will be

Proposition 3.3 *Let $r \geq 1$ be a fixed integer. We define the real function*

$$f(x_1, \ldots, x_r) := \sum_{k=1}^{r} \sum_{i=k}^{r} \prod_{j=k}^{i} x_j$$

for $(x_1, \ldots, x_r) \in [0, 1]^r$. Let $0 < \rho \leq 2^{-r}$. Then

$$\min \left\{ f(x_1, \ldots, x_r) : (x_1, \ldots, x_r) \in [0, 1]^r, \ x_1 \cdot x_2 \cdots x_r = \rho \right\} = (r + \mu(\rho, r)) \cdot \mu(\rho, r),$$

where $\mu(\rho, r) := \nu(\rho, r)/(1 - \nu(\rho, r))$ and $x = \nu(\rho, r)$ is the unique real solution of the equation $x^r = \rho(1 - x)^2$ on the interval $[0, 1]$. The minimum obviously equals ρ for $r = 1$, and it is $\rho + 2\sqrt{\rho}$ for $r = 2$.
There is a unique minimizer for each r, namely

$$\begin{cases} \rho \in [0, 1] & \text{for } r = 1, \\ (\mu(\rho, 2), \mu(\rho, 2)) \in [0, 1]^2 & \text{for } r = 2, \\ (\mu(\rho, r), \nu(\rho, r), \ldots, \nu(\rho, r), \mu(\rho, r)) \in [0, 1]^r & \text{for } r \geq 3. \end{cases}$$

In the special case $r = 2$, we have explicitly $\mu(\rho, 2) = \sqrt{\rho}$.

PROOF. For $r \leq 2$, we have to deal with nothing more than quadratic equations, and in these cases all assertions follow easily from standard analysis.

For $r \geq 3$, we use the method of Lagrange multipliers to obtain necessary conditions for local minima of $f(x_1, \ldots, x_r)$ subject to the constraint $x_1 \cdot x_2 \cdots x_r = \rho$. Accordingly, let

$$F(x_1, \ldots, x_r, \lambda) := f(x_1, \ldots, x_r) + \lambda(\rho - x_1 \cdot x_2 \cdots x_r).$$

A necessary condition for a local minimum is that all partial derivatives $F_{x_t} := \frac{\partial F}{\partial x_t}$ $(1 \leq t \leq r)$ as well as $F_\lambda := \frac{\partial F}{\partial \lambda}$ vanish at that point. We have for $1 \leq t \leq r$

$$\begin{aligned} f_{x_t}(x_1, \ldots, x_r) &= \sum_{k=1}^{r} \sum_{i=k}^{r} \frac{\partial}{\partial x_t} \left(\prod_{j=k}^{i} x_j \right) \\ &= \sum_{k=1}^{\min\{r,t\}} \sum_{i=\max\{k,t\}}^{r} \frac{\partial}{\partial x_t} \left(\prod_{j=k}^{i} x_j \right) = \sum_{k=1}^{t} \sum_{i=t}^{r} \prod_{\substack{j=k \\ j \neq t}}^{i} x_j. \end{aligned}$$

Hence

$$x_t F_{x_t} = x_t f_{x_t}(x_1, \ldots, x_r) - x_t \left(\lambda \prod_{\substack{j=1 \\ j \neq t}}^{r} x_j \right) = \sum_{k=1}^{t} \sum_{i=t}^{r} \prod_{j=k}^{i} x_j - \lambda \rho,$$

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and we want to find all solutions $(x_1, \ldots, x_r)$ of the following system of equations:

$$\begin{cases} \displaystyle\sum_{k=1}^{t}\sum_{i=t}^{r}\prod_{j=k}^{i} x_j = \lambda\rho & (1 \le t \le r)\,, \\[2ex] x_1 \cdots x_r = \rho\,. \end{cases} \tag{9}$$

From now on we consider r and ρ to be fixed and abbreviate $\mu := \mu(\rho, r)$ and $\nu := \nu(\rho, r)$.

<u>Claim</u>: One solution of (9) is given by $x_1 = x_r = \mu$ and $x_2 = \ldots = x_{r-1} = \nu$, where we have $0 < \nu < \mu < 1$.

The real function $h(x) := x^r - \rho(1-x)^2$ is strictly increasing on the interval $[0,1]$ with $h(0) = -\rho$ and $h(1) = 1$. Hence $x^r = \rho(1-x)^2$ has a unique solution on $(0,1)$, which is denoted by ν. Since $\nu^r < \rho < 2^{-r}$, we even know $\nu < 1/2$. This implies $\nu < \mu < 1$.

In order to show that $(\mu, \nu, \nu, \ldots, \nu, \mu) \in (0,1)^r$ satisfies (9), we separate terms containing x_1 or x_r from the others in the double sum of (9) and obtain for $x_1 = x_r = \mu$ and $x_2 = \ldots = x_{r-1} = \nu$

$$\begin{aligned}
\sum_{k=1}^{t}\sum_{i=t}^{r}\prod_{j=k}^{i} x_j &= x_1 \cdots x_r + \sum_{i=t}^{r-1}\prod_{j=1}^{i} x_j + \sum_{k=2}^{t}\prod_{j=k}^{r} x_j + \sum_{k=2}^{t}\sum_{i=t}^{r-1}\prod_{j=k}^{i} x_j \\[1ex]
&= \rho + \sum_{i=t}^{r-1}\mu\cdot\nu^{i-1} + \sum_{k=2}^{t}\nu^{r-k}\cdot\mu + \sum_{k=2}^{t}\sum_{i=t}^{r-1}\nu^{i-k+1} \\[1ex]
&= \rho + \mu\cdot\frac{\nu^{t-1}-\nu^{r-1}}{1-\nu} + \mu\cdot\frac{\nu^{r-t}-\nu^{r-1}}{1-\nu} + \sum_{k=2}^{t}\frac{\nu^{t-k+1}-\nu^{r-k+1}}{1-\nu} \\[1ex]
&= \rho + \mu\cdot\frac{\nu^{t-1}-2\nu^{r-1}+\nu^{r-t}}{1-\nu} + \frac{1}{1-\nu}\left(\frac{\nu-\nu^{t}}{1-\nu} - \frac{\nu^{r-t+1}-\nu^{r}}{1-\nu}\right) \\[1ex]
&= \rho + \frac{1}{(1-\nu)^2}\left(\mu(1-\nu)(\nu^{t-1}-2\nu^{r-1}+\nu^{r-t}) + (\nu-\nu^{t}-\nu^{r-t+1}+\nu^{r})\right).
\end{aligned}$$

Since $\mu(1-\nu) = \nu$, we conclude for $(x_1, \ldots, x_r) = (\mu, \nu, \ldots, \nu, \mu)$ that

$$\sum_{k=1}^{t}\sum_{i=t}^{r}\prod_{j=k}^{i} x_j = \rho + \frac{\nu\cdot(1-\nu^{r-1})}{(1-\nu)^2} = \frac{\rho}{\nu^{r-1}}\,.$$

Setting $\lambda := 1/\nu^{r-1}$, this reveals that $(\mu, \nu, \ldots, \nu, \mu)$ satisfies all the upper equations in (9). The observation that

$$x_1 \cdots x_r = \mu^2\cdot\nu^{r-2} = \frac{\nu^{r}}{(1-\nu)^2} = \rho$$

completes the proof of the claim.

We now want to show that $f(\mu, \nu, \ldots, \nu, \mu)$ is in fact a minimum subject to the constraint $x_1 \cdot x_2 \cdots x_r = \rho$, and we shall see as well that $(\mu, \nu, \ldots, \nu, \mu)$ is the unique minimizer. By Proposition 3.1(i) the function $g_2(y_1, \ldots, y_r) = f(2^{-y_1}, \ldots, 2^{-y_r})$ is strictly convex for all

$(y_1, \ldots, y_r) \in \mathbb{R}^r$. Our claim has shown that $(\mu, \nu, \ldots, \nu, \mu)$ is an extremal point of f on the set $\{(x_1, \ldots, x_r) \in [0,1]^r : x_1 \cdots x_r = \rho\}$. Therefore $(\mu', \nu', \ldots, \nu', \mu')$ with

$$\mu' := \frac{\log(1/\mu)}{\log 2} \quad \text{and} \quad \nu' := \frac{\log(1/\nu)}{\log 2}$$

is an extremal point of g_2 on the set

$$U := \{(y_1, \ldots, y_r) \in \mathbb{R}^r_{\geq 0} : 2^{-y_1} \cdots 2^{-y_r} = \rho\} = \{(y_1, \ldots, y_r) \in \mathbb{R}^r_{\geq 0} : y_1 + \ldots + y_r = \sigma\},$$

where

$$\sigma := \frac{\log(1/\rho)}{\log 2} \geq r.$$

The set U apparently is the simplex with vertices $(\sigma, 0, \ldots, 0), (0, \sigma, 0, \ldots, 0), \ldots, (0, \ldots, 0, \sigma)$, and therefore a convex subset of $\mathbb{R}^r_{\geq 0}$. It is immediately clear that $(\mu', \nu', \ldots, \nu', \mu')$ does not lie on the boundary of the simplex U, in other words: the point belongs to the set U^0 of inner points of U. Altogether the function g_2 is strictly convex on the open convex set U^0 and $(\mu', \nu', \ldots, \nu', \mu')$ is an extremal point of g_2 in U^0. By Proposition 3.2(i) this point $(\mu', \nu', \ldots, \nu', \mu')$ is a minimal point of g_2, and by Proposition 3.2(ii) it is unique. Since $\log_2$ is strictly monotonic, the point $(\mu, \nu, \ldots, \nu, \mu)$ is the unique minimizer with respect to f on $\{(x_1, \ldots, x_r) \in [0,1]^r : x_1 \cdots x_r = \rho\}$.

It remains to calculate the minimum. We obtain similarly as before

$$f(x_1, \ldots, x_r) = x_1 \cdots x_r + \sum_{i=1}^{r-1} \prod_{j=1}^{i} x_j + \sum_{k=2}^{r} \prod_{j=k}^{r} x_j + \sum_{k=2}^{r-1} \sum_{i=k}^{r-1} \prod_{j=k}^{i} x_j.$$

By evaluating the geometric sums and using the identity $\mu = \nu/(1-\nu)$, it follows that

$$\begin{aligned}
f(\mu, \nu, \ldots, \nu, \mu) &= \mu^2 \nu^{r-2} + 2\mu \cdot \frac{1 - \nu^{r-1}}{1 - \nu} + \frac{1}{1 - \nu}\left((r-2)\nu - \frac{\nu^2 - \nu^r}{1 - \nu}\right) \\
&= \frac{\nu^r}{(1-\nu)^2} + \frac{2\nu(1 - \nu^{r-1})}{(1-\nu)^2} + \frac{\nu}{1-\nu} \cdot (r-2) - \frac{\nu^2 - \nu^r}{(1-\nu)^2} \\
&= \frac{2\nu - \nu^2}{(1-\nu)^2} + \frac{\nu}{1-\nu} \cdot (r-2) \\
&= \frac{2\nu}{1-\nu} + \frac{\nu^2}{(1-\nu)^2} + \frac{\nu}{1-\nu} \cdot (r-2) \\
&= 2\mu + \mu^2 + \mu(r-2) = (r + \mu) \cdot \mu.
\end{aligned}$$

$\square$

Corollary 3.2 *Let p be a prime and $r \geq 2$ an integer. For a given real number $\sigma \geq (r-1)\log 2/\log p$ let $x = \tilde{\nu}_p(\sigma, r)$ be the unique real solution of the equation $p^\sigma x^{r-1} = (1-x)^2$ on the interval $[0,1]$, and $\tilde{\mu}_p(\sigma, r) := \tilde{\nu}_p(\sigma, r)/(1 - \tilde{\nu}_p(\sigma, r))$. Then*

$$\tilde{m}_p(\sigma, r) = (r - 1 + \tilde{\mu}_p(\sigma, r)) \cdot \tilde{\mu}_p(\sigma, r),$$

and this value is exclusively attained by $h_p(\alpha_1, \ldots, \alpha_r)$ *for* $\alpha_j = \alpha_j(\sigma, r)$ *($1 \le j \le r$) defined as* $\alpha_1(\sigma, r) := 0$, $\alpha_r(\sigma, r) := \sigma$ *and*

$$\alpha_j(\sigma, r) := \frac{\log\left(\tilde{\mu}_p(\sigma, r)^{-1}\right)}{\log p} + (j-2)\frac{\log\left(\tilde{\nu}_p(\sigma, r)^{-1}\right)}{\log p} \qquad (r \ge 3;\ 2 \le j \le r-1). \qquad (10)$$

PROOF. Let $0 \le \alpha_1 \le \alpha_2 \le \ldots \le \alpha_r \le \sigma$ be arbitrary, and set $y_j := \alpha_{j+1} - \alpha_j$ for $1 \le j \le r-1$. Hence $\alpha_i - \alpha_k = y_k + y_{k+1} + \ldots + y_{i-1}$ for $1 \le k < i \le r$. This implies

$$\begin{aligned}
h_p(\alpha_1, \ldots, \alpha_r) &= \sum_{k=1}^{r-1} \sum_{i=k+1}^{r} \frac{1}{p^{y_k + \ldots + y_{i-1}}} \\
&= \sum_{k=1}^{r-1} \sum_{i=k+1}^{r} \prod_{j=k}^{i-1} \frac{1}{p^{y_j}} = \sum_{k=1}^{r-1} \sum_{i=k}^{r-1} \prod_{j=k}^{i} \frac{1}{p^{y_j}}.
\end{aligned}$$

On setting $x_j := p^{-y_j}$ for $1 \le j \le r-1$, we have $h_p(\alpha_1, \ldots, \alpha_r) = f(x_1, \ldots, x_{r-1})$ for the function f as defined in Proposition 3.3. By hypothesis, $r - 1 \ge 1$ and $(x_1, \ldots, x_{r-1}) \in [0, 1]^{r-1}$. Now we search for conditions to be imposed on the α_j in order to hit the minimum $\tilde{m}_p(\sigma, r)$. First of all, we necessarily have $\alpha_1 = 0$ and $\alpha_r = \sigma$ according to (7). Hence

$$x_1 \cdot x_2 \cdot \ldots \cdot x_{r-1} = \frac{1}{p^{y_1 + \ldots + y_{r-1}}} = \frac{1}{p^{\alpha_r - \alpha_1}} = \frac{1}{p^{\sigma}}.$$

Again by hypothesis

$$0 < \rho := \frac{1}{p^{\sigma}} \le \frac{1}{2^{r-1}}.$$

Applying Proposition 3.3, we conclude that

$$\tilde{m}_p(\sigma, r) = (r - 1 + \mu(\rho, r-1)) \cdot \mu(\rho, r-1) = (r - 1 + \tilde{\mu}_p(\sigma, r)) \cdot \tilde{\mu}_p(\sigma, r),$$

where this minimum is exclusively obtained for $x_1 = x_{r-1} = \tilde{\mu}_p(\sigma, r)$ and $x_2 = x_3 = \ldots = x_{r-2} = \tilde{\nu}_p(\sigma, r)$. This yields for the given values of the x_j

$$\frac{1}{p^{\alpha_2}} = \frac{1}{p^{\alpha_2 - \alpha_1}} = \frac{1}{p^{y_1}} = x_1 = \tilde{\mu}_p(\sigma, r),$$

hence $\alpha_2 = \log(1/\tilde{\mu}_p(\sigma, r))/\log p$, and for $2 \le j \le r-2$

$$\frac{1}{p^{\alpha_{j+1} - \alpha_j}} = \frac{1}{p^{y_j}} = x_j = \tilde{\nu}_p(\sigma, r),$$

which implies (10). □

4 Integral circulant graphs with maximal energy

Up to this point, all we have done with respect to general integral circulant graphs with maximal energy refers to *real* parameters α_j in $h_p(\alpha_1, \ldots, \alpha_r)$. As a consequence, we have the following upper bound for $\mathcal{E}_{\max}(p^s, r)$, but we are left with the task to find out how close we can get to the "real maximum" if we restrict ourselves to *integral* parameters $a_1, \ldots, a_r$, as required by our problem.

Theorem 4.1 *For a prime p and integers $2 \le r \le s$, we have*

$$\mathcal{E}_{\max}(p^s, r) \le 2(p-1)p^{s-1}\Big(r - (p-1)\big(r - 1 + \tilde{\mu}_p(s-1, r)\big)\tilde{\mu}_p(s-1, r)\Big),$$

where $\tilde{\mu}_p$ is defined in Corollary 3.2.

PROOF.   By Corollary 3.2 and the definitions of $m_p(s-1, r)$ and $\tilde{m}_p(\sigma, r)$, we immediately have for any integer $s \ge r - 1$

$$m_p(s - 1, r) \ge (r - 1 + \tilde{\mu}_p(s - 1, r)) \cdot \tilde{\mu}_p(s - 1, r).$$

Now our theorem follows at once from this and (4). □

The first step we take towards integrality of the parameters is to approximate the numbers $\tilde{\mu}_p(s - 1, r)$, $\tilde{\nu}_p(s - 1, r)$ and the corresponding $\alpha_j(s - 1, r)$, all defined in Corollary 3.2, by simpler terms.

Proposition 4.1 *For a prime p and integers $3 \le r \le s$, let $\delta := p^{-\frac{s-1}{r-1}}$. Then we have*

(i) $\delta \le \tilde{\mu}_p(s - 1, r) < \delta + \frac{\delta^2}{1-\delta}$;

(ii) $\delta - \frac{\delta^2}{1+\delta} \le \tilde{\nu}_p(s - 1, r) < \delta \le \frac{1}{p}$;

(iii) $0 < \log\big(\tilde{\nu}_p(s - 1, r)^{-1}\big) - \frac{s-1}{r-1}\log p < \frac{3}{(r-1)p}$;

(iv) $-\frac{3}{2p} < \log\big(\tilde{\mu}_p(s - 1, r)^{-1}\big) - \frac{s-1}{r-1}\log p \le 0$;

(v) $|\alpha_j(s - 1, r) - (j - 1)\frac{s-1}{r-1}| < \frac{3}{p\log p}$ *for* $1 \le j \le r$.

PROOF.   (i) It follows from the definition of $\tilde{\mu} := \tilde{\mu}_p(s - 1, r)$ in Corollary 3.2 that it satisfies the identity $p^{s-1}\tilde{\mu}^{r-1} = (1 + \tilde{\mu})^{r-3}$, clearly implying $0 < \tilde{\mu} < 1$. For $r = 3$, this means that $\tilde{\mu} = \delta$. For $r \ge 4$, we obtain by virtue of binomial expansion

$$\tilde{\mu} = \delta(1 + \tilde{\mu})^{\frac{r-3}{r-1}} = \delta + \delta \sum_{k=1}^{\infty} \binom{\frac{r-3}{r-1}}{k} \tilde{\mu}^k,$$

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where the infinite series has alternating decreasing terms. Hence

$$0 < \tilde{\mu} - \delta < \delta \cdot \frac{r-3}{r-1} \cdot \tilde{\mu} < \delta\tilde{\mu},$$

and consequently $\tilde{\mu} < \delta/(1-\delta)$, which implies (i).

(ii) Since the real function $x \mapsto x/(1+x)$ is strictly increasing for $x > 0$, we obtain by (i)

$$\delta - \frac{\delta^2}{1+\delta} = \frac{\delta}{1+\delta} \leq \frac{\tilde{\mu}}{1+\tilde{\mu}} < \frac{\delta + \frac{\delta^2}{1-\delta}}{1+\delta+\frac{\delta^2}{1-\delta}} = \delta.$$

The definition in Corollary 3.2 yields that $\tilde{\nu} := \tilde{\nu}_p(s-1,r) = \tilde{\mu}/(1+\tilde{\mu})$, which proves our claim.

(iii) By (ii), we have $0 < \tilde{\nu} < \frac{1}{p}$. Taking logarithms in the identity $p^{s-1}\tilde{\nu}^{r-1} = (1-\tilde{\nu})^2$ (cf. Cor. 3.2), we obtain

$$\log\frac{1}{\tilde{\nu}} = \frac{s-1}{r-1}\log p - \frac{2}{r-1}\log(1-\tilde{\nu}). \tag{11}$$

Since $\tilde{\nu} < 1/p$, the Taylor expansion of $\log(1-\tilde{\nu})$ yields

$$0 < -\log(1-\tilde{\nu}) = \sum_{k=1}^{\infty}\frac{\tilde{\nu}^k}{k} < \tilde{\nu} + \frac{\tilde{\nu}^2}{2}\sum_{k=0}^{\infty}\tilde{\nu}^k = \tilde{\nu} + \frac{\tilde{\nu}^2}{2(1-\tilde{\nu})} < \frac{3}{2}\tilde{\nu} < \frac{3}{2p}.$$

Inserting this into (11), we get

$$0 < \log\frac{1}{\tilde{\nu}} - \frac{s-1}{r-1}\log p < \frac{3}{(r-1)p}.$$

(iv) For the numbers $\alpha_j := \alpha_j(s-1,r)$, as defined for $1 \leq j \leq r$ in Corollary 3.2, we have

$$\alpha_{j+1} - \alpha_j = \begin{cases} \frac{\log(1/\tilde{\mu})}{\log p} & \text{for } j = 1 \text{ and } j = r-1, \\ \frac{\log(1/\tilde{\nu})}{\log p} & \text{for } 2 \leq j \leq r-2. \end{cases} \tag{12}$$

This is trivial except for $j = r-1$, where it follows from the identities $\tilde{\mu} = \tilde{\nu}/(1-\tilde{\nu})$ and $p^{s-1}\tilde{\nu}^{r-1} = (1-\tilde{\nu})^2$. Therefore,

$$s - 1 = \alpha_r - \alpha_1 = \sum_{j=1}^{r-1}(\alpha_{j+1} - \alpha_j) = \frac{2\log(1/\tilde{\mu})}{\log p} + \frac{(r-3)\log(1/\tilde{\nu})}{\log p},$$

hence

$$\log\frac{1}{\tilde{\mu}} - \frac{s-1}{r-1}\log p = \frac{r-3}{2}\left(\frac{s-1}{r-1}\log p - \log\frac{1}{\tilde{\nu}}\right).$$

Combining this with the bounds found in (iii) completes the argument.

(v) By the definition of the α_j, we obtain for $2 \leq j \leq r-1$

$$\alpha_j(s-1,r) - (j-1)\frac{s-1}{r-1} = \left(\frac{\log\frac{1}{\tilde{\mu}}}{\log p} - \frac{s-1}{r-1}\right) + (j-2)\left(\frac{\log\frac{1}{\tilde{\nu}}}{\log p} - \frac{s-1}{r-1}\right).$$

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From (iii) and (iv) it follows that

$$-\frac{3}{2p\log p} < \alpha_j(s-1,r) - (j-1)\frac{s-1}{r-1} < (j-2)\frac{3}{(r-1)p\log p} < \frac{3}{p\log p},$$

which implies (v) in these cases. Since $\alpha_1 = 0$ and $\alpha_r = s - 1$, the inequality is valid for all j.

$\square$

Proposition 4.1(v) reveals that picking the α_j for $j = 1, \ldots, r$ well-spaced in the interval $[0, s-1]$, i.e. $\alpha_j := (j-1)\frac{s-1}{r-1}$ (see concluding remarks of section 2), is close to best possible. Since it is our task to find *integral* a_j in optimal position, it suggests itself to choose the a_j as nearest integers to the $\alpha_j(s-1, r)$ (as defined in Corollary 3.2) or to the numbers $(j-1)\frac{s-1}{r-1}$, which does not make much of a difference by Proposition 4.1(v). Anyway, we shall take $a_j = \|\alpha_j\|$ ($1 \le j \le r$) with the nearest integer function $\|\cdot\|$ and have to accept variations between α_j and a_j in the range from $-\frac{1}{2}$ to $\frac{1}{2}$. Finally, we shall try to maximize the energy with respect to r.

We now show that our *integral minimum* $m_p(s-1, r)$, as defined in (3), can be bounded by the *real minimum* $\tilde{m}_p(s-1, r)$, introduced in (6). In general, that is to say in worst cases, we cannot expect to lose less than a factor p between the two minima, taking into account that the shifts from real numbers α_j to integral parameters a_j, varying over an interval of length up to 1, have to be executed in h_p, i.e. in the exponent of p.

Proposition 4.2 *Let $3 \le r \le s$ be given integers, and let p be a prime.*

(i) *Let $(\alpha_1, \ldots, \alpha_r) \in \mathbb{R}^r$ be the unique minimizer of h_p determined in Cor. 3.2. Then $(a_1, \ldots, a_r) \in \mathbb{Z}^r$ with the nearest integers $a_j := \|\alpha_j\|$ ($1 \le j \le r$) has the property*

$$h_p(a_1, \ldots, a_r) \le \begin{cases} 4 \cdot \tilde{m}_2(s-1, r) & \text{for } p = 2, \\ p \cdot \tilde{m}_p(s-1, r) & \text{for } p \ge 3. \end{cases}$$

(ii) *We have* $\quad \tilde{m}_2(s-1, r) \le m_2(s-1, r) \le 4 \cdot \tilde{m}_2(s-1, r).$

(iii) *For any prime $p \ge 3$, we have*

$$\tilde{m}_p(s-1, r) \le m_p(s-1, r) \le p \cdot \tilde{m}_p(s-1, r).$$

PROOF.   The lower bounds in (ii) and (iii) are trivial, and the upper bounds follow immediately from the definition of $m_p(s-1, r)$ in (3). Hence it suffices to prove (i). By Corollary 3.2, we have $\alpha_j = \alpha_j(s-1, r)$ for $1 \le j \le r$ and

$$h_p(\alpha_1, \ldots, \alpha_r) = \tilde{m}_p(s-1, r).$$

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Since $\tilde{\nu} := \tilde{\nu}_p(s-1,r) < 1/p$ by Proposition 4.1(ii), we have $\log(1/\tilde{\nu}) \geq \log p$. From Proposition 4.1(i) it follows for $p \geq 3$ that $\tilde{\mu} := \tilde{\mu}_p(s-1,r) < 1/\sqrt{p}$, hence $\log(1/\tilde{\mu}) > \frac{1}{2}\log p$. By use of (12), these inequalities imply that $\alpha_2 > \frac{1}{2}$, $\alpha_{r-1} < s-1-\frac{1}{2}$ and $\alpha_{j+1} \geq \alpha_j + 1$ for $2 \leq j \leq r-2$. Moreover, $\alpha_1 = 0$ and $\alpha_r = s-1$. Therefore, the nearest integers $a_j := \|\alpha_j\|$, $1 \leq j \leq r$, are pairwise distinct, forming a strictly increasing sequence. We have $a_j = \alpha_j + \delta_j$ for suitable real numbers δ_j satisfying $|\delta_j| \leq 1/2$ $(1 \leq j \leq r)$ and obtain

$$
\begin{aligned}
h_p(a_1, \ldots, a_r) &= \sum_{k=1}^{r-1} \sum_{i=k+1}^{r} \frac{1}{p^{a_i - a_k}} \\
&= \sum_{k=1}^{r-1} \sum_{i=k+1}^{r} \frac{1}{p^{(\alpha_i - \delta_i)-(\alpha_k - \delta_k)}} = \sum_{k=1}^{r-1} \sum_{i=k+1}^{r} \frac{1}{p^{\delta_k - \delta_i}} \frac{1}{p^{\alpha_i - \alpha_k}} \\
&\leq p \sum_{k=1}^{r-1} \sum_{i=k+1}^{r} \frac{1}{p^{\alpha_i - \alpha_k}} = p \cdot \tilde{m}_p(s-1,r).
\end{aligned}
$$

For the prime $p = 2$ the above proof has to be modified, since possibly $\alpha_2 < \frac{1}{2}$. In this case we choose $a_2 = 1$ and $a_{r-1} = s-2$. As before, $\alpha_{j+1} \geq \alpha_j + 1$ for $2 \leq j \leq r-2$. Hence we can select each a_j, $3 \leq j \leq r-2$, as one of the neighbouring integers of α_j in such a way that $a_1 < a_2 < \ldots < a_r$. It follows in this case that $a_j = \alpha_j + \delta_j$ for suitable real numbers δ_j satisfying $|\delta_j| \leq 1$ $(1 \leq j \leq r)$. Consequently

$$
h_2(a_1, \ldots, a_r) = \sum_{k=1}^{r-1} \sum_{i=k+1}^{r} \frac{1}{2^{\delta_k - \delta_i}} \frac{1}{2^{\alpha_i - \alpha_k}} \leq 2^2 \sum_{k=1}^{r-1} \sum_{i=k+1}^{r} \frac{1}{2^{\alpha_i - \alpha_k}} = 4 \cdot \tilde{m}_2(s-1,r).
$$

$\square$

Remark. The factor p (or 4 in case $p = 2$, respectively) we lose between the *real minimum* $\tilde{m}_2(s-1,r)$ and the *integral minimum* $m_p(s-1,r)$ according to (ii) and (iii) reflects the hypothetical worst case scenario where each a_j differs from α_j by $\frac{1}{2}$. In practice, the factor between the two minima will be substantially smaller in almost all cases.

In Theorem 2.1 the maximal energy $\mathcal{E}_{\max}(p^s)$ as well as the corresponding p^s-maximal sets are given for all primes p and each $s \leq 4$, and could be determined quite easily for other small values of s by (2), i.e. Theorem 2.1 in [18]. The inequality

$$
\mathcal{E}^*_{\max}(p^s) := \frac{\mathcal{E}_{\max}(p^s)}{2(p-1)p^{s-1}} \leq s
$$

is an immediate consequence of Theorem 4.1. The following result shows that this trivial upper bound lies close to the true value of $\mathcal{E}^*_{\max}(p^s)$.

More precisely, part (ii) of the following Theorem 4.2 provides the explicit construction of a divisor set $\mathcal{D}_0$ such that the energy of the graph $\mathrm{ICG}(p^s, \mathcal{D}_0)$ falls short of the maximal

energy $\mathcal{E}_{\max}(p^s)$ among all integral circulant graphs of order p^s essentially by a factor less than 2. The remark preceding Proposition 4.2 explains why we cannot expect to find a more precise lower bound in general. However, the reader should be aware of the fact that we lose a much smaller factor than 2 between upper and lower bound for $\mathcal{E}_{\max}^*(p^s)$ in most cases (cf. the remark following Prop. 4.2). We shall comment on this at the end of the section.

Bound by the tradition of number theory, *log* will denote the natural logarithm.

Theorem 4.2 *Let p be a prime and let s be a positive integer.*

(i) We have

$$\underline{C} \cdot (s-1) \left(1 - \frac{\log\log p}{\log p}\right) \leq \mathcal{E}_{\max}^*(p^s) \leq \overline{C} \cdot (s-1) \left(1 - \frac{\log\log p}{\log p}\right) + 1, \qquad (13)$$

where $\overline{C} = 1$ for all $p \geq 3$ and $\underline{C} = \frac{1}{2}$ for all $p \geq 17$ as well as for $3 \leq p \leq 13$ in case $s \leq 6$. Only for small values of p, we have exceptional constants $\overline{C} = \overline{C}(p)$ and $\underline{C} = \underline{C}(p)$, namely $\overline{C}(2) = 0.328$, $\underline{C}(2) = 0.118$, and in case $s \geq 7$

$$\underline{C}(p) = \begin{cases} 0.030 & \text{if } p = 3, \\ 0.233 & \text{if } p = 5, \\ 0.337 & \text{if } p = 7, \\ 0.442 & \text{if } p = 11, \\ 0.473 & \text{if } p = 13. \end{cases}$$

(ii) Let r_0 be the integer uniquely determined by

$$\frac{s-1}{D(p)} \leq r_0 < \frac{s-1}{D(p)} + 1,$$

where

$$D(p) := \begin{cases} 4.09184 & \text{for } p = 2, \\ 2(1 + \frac{\log\log p}{\log p}) & \text{for } p \geq 3, \end{cases}$$

and define $\mathcal{D}_0 = \{p^{\|\alpha_j(s-1,r_0)\|} : j = 1, \ldots, r_0\}$. For $p = 2$, $s \geq 11$ and for $p \geq 3$, $s \geq 7$, the energy of the graph $\mathrm{ICG}(p^s, \mathcal{D}_0)$ lies in the same interval as the one established for $\mathcal{E}_{\max}(p^s)$ in (13).

PROOF. By Theorem 2.1 we have for all primes p

$$\mathcal{E}_{\max}^*(p^s) = \begin{cases} 1 & \text{for } s = 1, \\ 1 + \frac{1}{p} & \text{for } s = 2, \\ 2 - \frac{1}{p} + \frac{1}{p^2} & \text{for } s = 3, \\ 2 + \frac{1}{p^3} & \text{for } s = 4. \end{cases} \qquad (14)$$

We leave it to the reader to check that each of these values lies within the respective bounds stated in (13). We may therefore assume $s \geq 5$ in the sequel.

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We shall first prove the upper bound in (13). By virtue of (5), it suffices to show that

$$\frac{\mathcal{E}_{\max}(p^s, r)}{2(p-1)p^{s-1}} \le \overline{C} \cdot (s-1)\left(1 - \frac{\log\log p}{\log p}\right) + 1. \tag{15}$$

is satisfied for all $1 \le r \le s$. We distinguish three cases.

Case U1: $r = 1$.

By Corollary 2.1(i) in [18], we have $\mathcal{E}_{\max}(p^s, 1) = 2(p-1)p^{s-1}$ for all p, which implies (15) immediately.

Case U2: $r = 2$.

It follows from (4) and Proposition 2.1(i) that

$$\mathcal{E}_{\max}(p^s, 2) = 2(p-1)p^{s-1}\left(2 - (p-1)\frac{1}{p^{s-1}}\right) \tag{16}$$

for all p. Since $s \ge 5$, our upper bound in (15) is valid in this case.

Case U3: $3 \le r \le s$.

By Theorem 4.1 and Proposition 4.1(i), we have

$$\mathcal{E}_{\max}(p^s, r) \le 2(p-1)p^{s-1}\left(r - \frac{(p-1)(r-1)}{p^{\frac{s-1}{r-1}}}\right) \tag{17}$$

for all p. Therefore, we study for fixed p and s the real function

$$g(x) := x - \frac{(p-1)(x-1)}{p^{\frac{s-1}{x-1}}}$$

on the interval $3 \le x \le s$ with boundary values

$$g(3) = 3 - \frac{2(p-1)}{p^{\frac{s-1}{2}}} \quad \text{and} \quad g(s) = \frac{s-1}{p} + 1. \tag{18}$$

For a maximum of g at x_0, say, with $3 < x_0 < s$ the derivative

$$g'(x_0) = 1 - \frac{p-1}{p^{\frac{s-1}{x_0-1}}}\left(1 + \frac{(s-1)\log p}{x_0 - 1}\right)$$

vanishes necessarily. Substituting $y := \frac{s-1}{x-1}$, hence $y \ge 1$, we obtain the condition

$$1 + y_0 \log p = \frac{p^{y_0}}{p-1} \tag{19}$$

for $y_0 := \frac{s-1}{x_0-1}$. Since $x_0 = 1 + (s-1)/y_0$, we conclude for $3 \le x \le s$

$$g(x) \le g(x_0) = \frac{s-1}{y_0}\left(1 - \frac{p-1}{p^{y_0}}\right) + 1. \tag{20}$$

Case U3.1: $p = 2$.

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For $p = 2$, equation (19) has no solution $y_0 \geq 1$, i.e. in that case the maximum of g is attained at $y_0 = 1$, that is for $x_0 = s \geq 5$, which follows by comparison of the boundary values in (18). Therefore we have in case $p = 2$

$$g(x) \leq g(s) = s - \frac{s-1}{2} = \frac{s-1}{2} + 1.$$

By (17), this immediately implies (15).

Case U3.2: $p \geq 3$.

Now (19) has a unique solution y_0 in the interval $1 \leq y_0 < 2$, corresponding to the unique maximum of g. By a few steps of Newton interpolation we obtain for instance that $y_0 \approx 1.527$ for $p = 3$ and $y_0 \approx 1.673$ for $p = 5$. We shall verify that

$$g(x) \leq (s-1)\left(1 - \frac{\log\log p}{\log p}\right) + 1 \tag{21}$$

on the interval $3 \leq x \leq s$. This follows easily for $p = 3$ and $p = 5$ by inserting the respective values of y_0 given above into (20). For each other fixed prime $p \geq 7$, we define the real function

$$w(y) = w_p(y) := \frac{p^y}{p-1} - y\log p - 1$$

for all $y \geq 1$. By (19) we know that $y_0 \geq 1$ satisfies $w(y_0) = 0$. Since the derivative

$$w'(y) = \left(\frac{p^y}{p-1} - 1\right)\log p$$

is positive for $y \geq 1$, the function $w(y)$ is strictly increasing. For

$$y_p := \frac{\log p}{\log p - \log\log p} - \frac{1}{\log p},$$

which is greater than 1 for $p \geq 7$, we have

$$
\begin{aligned}
w(y_p) &= \frac{1}{p-1}p^{\frac{\log p}{\log p - \log\log p}} \cdot e^{-1} - \frac{(\log p)^2}{\log p - \log\log p} \\
&= \frac{1}{e(p-1)}p^{1 + \frac{\log\log p}{\log p - \log\log p}} - \frac{(\log p)^2}{\log p - \log\log p} \\
&< \frac{p}{e(p-1)}p^{\frac{\log\log p}{\log p - \log\log p}} - \log p < 0,
\end{aligned}
$$

where the final inequality is shown to hold for all primes $p \geq 7$ by simply taking logarithms in

$$\frac{p}{e(p-1)}p^{\frac{\log\log p}{\log p - \log\log p}} < \log p.$$

Since $w(y)$ is strictly increasing on $y \geq 1$ and $w(y_p) < 0$, but $w(y_0) = 0$, it follows that $y_p < y_0$. By definition of y_p, this inequality implies

$$\log p < \left(1 - \frac{\log\log p}{\log p}\right)(1 + y_0\log p).$$

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Multiplying with y_0 and dividing by $(1 + y_0 \log p)$, we obtain by (19)

$$1 - \frac{p-1}{p^{y_0}} = 1 - \frac{1}{1 + y_0 \log p} < y_0 \left(1 - \frac{\log\log p}{\log p}\right).$$

Inserting this into (20), we have verified (21). By (17), the proof of (15) is complete. Hence the upper bound in (13) holds in all cases.

Now we turn our attention to the lower bound for $\mathcal{E}^*_{\max}(p^s)$ an distinguish several cases and subcases.

Case L1: $p \geq 3$.
Case L1.1: $s \leq 4$.
The lower bound in (13) has already been verified for $s \leq 4$ in (14).
Case L1.2: $s = 5$.
Picking $r = 2$, we use (16) once more and obtain

$$\mathcal{E}^*_{\max}(p^5) \geq \frac{\mathcal{E}_{\max}(p^5, 2)}{2(p-1)p^4} = 2 - (p-1)\frac{1}{p^4} \geq 2\left(1 - \frac{\log\log p}{\log p}\right)$$

for all $p \geq 3$, which proves the lower bound of (13) in this case.
Case L1.3: $s = 6$.
It follows from (4) and Proposition 2.1(ii) that

$$\mathcal{E}^*_{\max}(p^6) \geq \frac{\mathcal{E}_{\max}(p^6, 3)}{2(p-1)p^5} = 3 - (p-1)\left(\frac{1}{p^2} + \frac{1}{p^5} + \frac{1}{p^3}\right) \geq \frac{5}{2}\left(1 - \frac{\log\log p}{\log p}\right)$$

for all $p \geq 3$, and again the lower bound in (13) is confirmed.
Case L1.4: $s \geq 7$.
We choose the integer r_0 according to the inequality

$$\frac{s-1}{2L_p} \leq r_0 < \frac{s-1}{2L_p} + 1, \tag{22}$$

where

$$L_p := 1 + \frac{\log\log p}{\log p}.$$

A simple calculation reveals that for $s \geq 7$ and all primes $p \geq 3$ the expression on the left-hand side of (22) is always greater than 2. Consequently, $3 \leq r_0 \leq s - 1$. By Corollary 3.2, we have

$$\tilde{m}_p(s-1, r_0) = (r_0 - 1 + \tilde{\mu}_p(s-1, r_0)) \cdot \tilde{\mu}_p(s-1, r_0), \tag{23}$$

and from Proposition 4.1(i) and the definition of r_0, we get $\tilde{\mu}_p(s-1, r_0) < \delta + \delta^2/(1-\delta)$ for $\delta = p^{-(s-1)/(r_0-1)} < p^{-2L_p}$. Hence

$$\tilde{\mu}_p(s-1, r_0) < \frac{1}{p^{2L_p}}\left(1 + \frac{1}{p^{2L_p} - 1}\right).$$

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By (23) and (22) we now have

$$\tilde{m}_p(s-1, r_0) \; < \; \left(\frac{s-1}{2L_p} + \frac{1}{p^{2L_p}} \left(1 + \frac{1}{p^{2L_p}-1} \right) \right) \cdot \frac{1}{p^{2L_p}} \left(1 + \frac{1}{p^{2L_p}-1} \right)$$

$$< \; \left(\frac{s-1}{2p^{2L_p}L_p} + \frac{1}{p^{4L_p}} \right) \cdot \frac{p}{p-1} \, ,$$

because for $p \geq 3$

$$1 + \frac{1}{p^{2L_p}-1} \; < \; \left(1 + \frac{1}{p^{2L_p}-1} \right)^2 = \left(1 + \frac{1}{p^2(\log p)^2 - 1} \right)^2$$

$$< \; \left(1 + \frac{1}{(p-1)(p+1)} \right)^2 < \frac{p}{p-1} \, .$$

Since $p \geq 3$, we obtain by Proposition 4.2(iii) that

$$m_p(s-1, r_0) \; < \; p \cdot \tilde{m}_p(s-1, r_0)$$

$$< \; \left(\frac{s-1}{2p^{2L_p}L_p} + \frac{1}{p^{4L_p}} \right) \cdot \frac{p^2}{p-1}$$

$$= \; \left(\frac{s-1}{2(\log p)^2 L_p} + \frac{1}{p^2(\log p)^4 L_p} \right) \cdot \frac{1}{p-1} \, .$$

According to (4) and (22), it follows that

$$\frac{\mathcal{E}_{\max}(p^s, r_0)}{2(p-1)p^{s-1}} \; = \; r_0 - (p-1)\, m_p(s-1, r_0)$$

$$> \; \frac{s-1}{2L_p} - \left(\frac{s-1}{2(\log p)^2 L_p} + \frac{1}{p^2(\log p)^4} \right) \tag{24}$$

$$> \; \frac{s-1}{2L_p} \left(1 - \frac{1}{(\log p)^2} \right) - \frac{1}{p^2(\log p)^4} \, .$$

It is easy to check that for all primes $p \geq 17$

$$(\log \log p)^2 > 1 + \frac{L_p}{3(p \log p)^2},$$

and that for $3 \leq p \leq 13$

$$(\log \log p)^2 > 1 + \left(\frac{1}{3(p \log p)^2} - c_p(\log p)^2 \right) L_p$$

with constants c_p defined by the following table:

p	c_p
3	0.859
5	0.375
7	0.214
11	0.073
13	0.033

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Setting $c_p := 0$ for all primes $p \geq 17$, the fact that $s \geq 7$ implies for all $p \geq 3$

$$(\log \log p)^2 + c_p \log p \, L_p > 1 + \frac{L_p}{3(p \log p)^2} \geq 1 + \frac{2L_p}{(s-1)(p \log p)^2}.$$

Dividing by $(\log p)^2$, adding 1 on both sides and rearranging terms yields

$$\begin{aligned}
1 - \frac{1}{(\log p)^2} - \frac{2L_p}{(s-1)p^2(\log p)^4} \; &> \; 1 - \left(\frac{\log \log p}{\log p}\right)^2 - \frac{c_p L_p}{\log p} \\
&= \; \left(1 - \frac{\log \log p}{\log p}\right) L_p - \frac{c_p L_p}{\log p}.
\end{aligned}$$

Dividing by L_p and multiplying with $(s-1)/2$ implies

$$\frac{s-1}{2L_p}\left(1 - \frac{1}{(\log p)^2}\right) - \frac{2}{(s-1)p^2(\log p)^4} > \frac{s-1}{2}\left(1 - \frac{\log \log p + c_p}{\log p}\right).$$

Inserting this inequality into (24) yields

$$\frac{\mathcal{E}_{\max}(p^s, r_0)}{2(p-1)p^{s-1}} > \frac{s-1}{2}\left(1 - \frac{\log \log p + c_p}{\log p}\right),$$

which completes the proof of the lower bound in (13) for $p \geq 3$. At the same time, our construction combined with Proposition 4.2(i) reveals the truth of statement (ii) for primes $p \geq 3$ and $s \geq 7$.

Case L2: $p = 2$.
Case L2.1: $s \leq 4$.
The lower bound in (13) follows from (14).
Case L2.2: $5 \leq s \leq 10$.
Picking $r = 3$, it follows from (4) and Proposition 2.1(ii) that

$$\mathcal{E}^*_{\max}(2^s) \geq \frac{\mathcal{E}_{\max}(2^s, 3)}{2^s} = 3 - \left(\frac{1}{2^{\lceil \frac{s-1}{2} \rceil}} + \frac{1}{2^{s-1}} + \frac{1}{2^{s-1-\lceil \frac{s-1}{2} \rceil}}\right).$$

It is easy to check that the last term becomes minimal for $s = 5$. Hence

$$\mathcal{E}^*_{\max}(2^s) \geq 3 - \frac{9}{16} \geq \frac{2}{11}(s-1)$$

for all s in the given range. This confirms the lower bound in (13) for these values of s.
Case L2.3: $s \geq 11$.
Let $c_1 > 1$ be the unique real number satisfying $c_1^2 - 6c_1 + 5 = 4c_1 \log c_1$, i.e. $17.0517 < c_1 < 17.0518$, and let $c_2 := \frac{\log c_1}{\log 2}$, thus $4.09184 < c_2 < 4.09186$. We choose the integer r_2 according to the inequality

$$\frac{s-1}{c_2} \leq r_2 < \frac{s-1}{c_2} + 1. \tag{25}$$

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Apparently, the expression on the left-hand side of (25) is always greater than 2 for $s \geq 11$. Consequently, $3 \leq r_2 \leq s - 1$. By Corollary 3.2, we have

$$\tilde{m}_2(s - 1, r_2) = (r_2 - 1 + \tilde{\mu}_p(s - 1, r_2)) \cdot \tilde{\mu}_p(s - 1, r_2), \tag{26}$$

and from Proposition 4.1(i) and the definition of r_2, we get

$$\tilde{\mu}_p(s - 1, r_2) < \frac{1}{2^{c_2}} + \frac{1}{2^{2c_2} - 2^{c_2}} = \frac{1}{2^{c_2}} \left(1 + \frac{1}{2^{c_2} - 1} \right).$$

By (26) and (25) we obtain

$$\tilde{m}_2(s - 1, r_2) < \left(\frac{s - 1}{c_2} + \frac{1}{2^{c_2}} \left(1 + \frac{1}{2^{c_2} - 1} \right) \right) \cdot \frac{1}{2^{c_2}} \left(1 + \frac{1}{2^{c_2} - 1} \right).$$

Proposition 4.2(ii) implies that $m_2(s - 1, r_2) < 4 \cdot \tilde{m}_2(s - 1, r_2)$, and with (4) and (25) we get

$$
\begin{aligned}
\mathcal{E}_{\max}^*(2^s) & \geq \frac{\mathcal{E}_{\max}(2^s, r_2)}{2^s} = r_2 - m_2(s - 1, r_2) \\
& > \frac{s - 1}{c_2} - 4 \left(\frac{s - 1}{c_2} + \frac{1}{2^{c_2}} \left(1 + \frac{1}{2^{c_2} - 1} \right) \right) \cdot \frac{1}{2^{c_2}} \left(1 + \frac{1}{2^{c_2} - 1} \right) \\
& = \frac{s - 1}{c_2} \left(1 - \frac{4}{2^{c_2}} \left(1 + \frac{1}{2^{c_2} - 1} \right) \right) - \frac{4}{2^{2c_2}} \left(1 + \frac{1}{2^{c_2} - 1} \right)^2 \\
& > \frac{s - 1}{5.45} - 0.01553 > \frac{2}{11}(s - 1)
\end{aligned}
$$

for $s \geq 11$. This proves the lower bound of (13) and completes part (i) of Theorem 4.2. This time our construction combined with Proposition 4.2(i) shows (ii) for $p = 2$ and $s \geq 11$.

$\square$

As an example, the following table illustrates the previous theorem for $s = 17$ and several small values of p. Note that r_0 will eventually become 8, roughly for $p > 10^{10}$).

n	r_0	$\mathcal{D}_0$	lower	$\mathcal{E}_{\max}^*(n)$	upper
3^{17}	8	$(0, 2, 5, 7, 9, 11, 14, 16)$	0.439	6.652	15.630
5^{17}	7	$(0, 3, 5, 8, 11, 13, 16)$	2.626	6.547	12.269
7^{17}	6	$(0, 3, 6, 10, 13, 16)$	3.547	5.927	11.526
11^{17}	6	$(0, 3, 6, 10, 13, 16)$	4.493	5.969	11.164
13^{17}	6	$(0, 3, 6, 10, 13, 16)$	4.789	5.978	11.124
17^{17}	6	$(0, 3, 6, 10, 13, 16)$	5.059	5.987	11.119
23^{17}	6	$(0, 3, 6, 10, 13, 16)$	5.084	5.993	11.169

Remarks.

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(i) The proof of Theorem 4.2 shows that we lose a factor 2 between lower and upper bound for $\mathcal{E}^*_{\max}(p^s)$ in case $p \geq 17$ (and similarly for smaller p) mainly due to the fact that we lose a factor p between $\tilde{m}_p(s-1, r)$ and $m_p(s-1, r)$, which however happens only as an extremely rare worst case event (cf. Proposition 4.2 and the preceding and subsequent remarks). A staightforward adaptation of the method introduced in the proof for the lower bound of (13) implies the following:

Assume that for some fixed sufficiently large p and s we have $m_p(s-1, r) \leq p^\gamma \cdot \tilde{m}_p(s-1, r)$ with some positive $\gamma < 1$. Taking

$$\frac{s+1}{(1+\gamma)L_p} \leq r_0 < \frac{s+1}{(1+\gamma)L_p} + 1$$

instead of (25), we obtain

$$\frac{1}{1+\gamma}(s+1)\left(1 - \frac{\log\log p}{\log p}\right) \leq \mathcal{E}^*_{\max}(p^s) \leq (s+1)\left(1 - \frac{\log\log p}{\log p}\right) + 1.$$

This reveals that, the smaller the difference between integral and real maximum is, the better our bounds are. In the extreme case where $m_p(s-1, r) = \tilde{m}_p(s-1, r)$, i.e. $\gamma = 0$, lower and upper bound differ only by 1, and the gcd graph with the corresponding divisor set $\mathcal{D}_0$ has maximal energy, because the energy is an integral number, but the two bounds are not.

(ii) It should be noted that even the lower bound of (13) already implies hyperenergeticity in most cases. A straightforward calculation shows this for e.g. $p \geq 3$ and $s \geq 5$.

5   Conclusion and open problems

Given a fixed prime power p^s, we have provided a method to construct a divisor set $\mathcal{D}_0$ with the property that $\mathcal{E}(p^s, \mathcal{D}_0) \geq \frac{1}{2}\mathcal{E}_{\max}(p^s)$. In most cases we expect $\mathcal{E}(p^s, \mathcal{D}_0)$ to lie much closer to $\mathcal{E}_{\max}(p^s)$ than our worst case inequality guarantees. But since we have used the "real" maximum for reference it may not be expected to get hold of the "integral" maximum in general, using an analytic approach. The convexity properties of the function h_p also suggest that a divisor set $\mathcal{D}_{\max}$ with $\mathcal{E}(p^s, \mathcal{D}_{\max}) = \mathcal{E}_{\max}(p^s)$ can be found in the "neighborhood" of our $\mathcal{D}_0$. Given an explicit integer p^s it should not be too difficult to determine $\mathcal{E}_{\max}(p^s)$ precisely by comparison of a few candidates for a $\mathcal{D}_{\max}$ "near" $\mathcal{D}_0$.

Let us conclude this section by posing the challenge of finding similarly accessible bounds on $\mathcal{E}_{\max}(n)$ for integers n which have different prime factors. Even for $n = p_1^{s_1} p_2^{s_2}$ with primes $p_1 \neq p_2$ and arbitrary divisor sets a closed formula for the energy of the corresponding integral circulant graphs would be most desirable. Of course, this should then be the basis for analyzing these graphs for hyperenergeticity.

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